

# Spatial Discretization in NIMROD

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and the NIMROD Team

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## MEMBERS OF THE NIMROD TEAM

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Olivier Sauter	ITER	Customer
Ming Chu	General Atomics	Customer
Alan Turnbull	General Atomics	Customer
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## Spatial Discretization in NIMROD

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NIMROD studies the nonlinear evolution of long-wavelength tokamak instabilities, with long time scales, requiring an implicit time step; and strong anisotropy and near-singular mode structure, requiring high spatial resolution. Toroidal discretization is pseudospectral. Multiple grid blocks are used in the poloidal plane, allowing for efficient parallelization, and for specialized methods each designed for a specific subdomain. The plasma region uses logically rectangular grid blocks based on non-orthogonal flux coordinates, infrequently updated to track the axisymmetric component of the magnetic field. This region is broken into annular zones to minimize coupling among blocks. Bilinear finite elements are used to avoid the need for staggered grids, required by finite-volume methods to ensure proper vector annihilation properties. Metric quantities are fit to bicubic splines for greater smoothness. A scrape-off layer uses a grid-block of adaptive, unstructured triangles. The vacuum region uses cylindrical coordinates. Small grid patches in the neighborhood of the o-point and the x-point can be used to avoid numerical difficulties caused by the coordinate system singularities.

## KEY FEATURES OF NIMROD

- Designed to study mode-locking and disruptions; low- $n$ , global, separatrix, resistive wall; nonlinear, time-dependent, realistic geometry and dynamics.
- Nation-wide collaboration, using **Integrated Product Development** (IPD) and **Quality Function Deployment** (QFD).
- Graphic pre-processor, solver, and graphic post-processor all controlled by **Graphical User Interface** (GUI).
- **Object-Oriented Programming** (OOP) using Fortran 90 for solver.
- Physics based on Quiet Implicit Pic (QIP) model: 2-fluid +  $\delta f$  particles + Maxwell. Braginskii++
- Spatial discretization uses multiple grid blocks, both logically rectangular and unstructured triangular. Finite elements, flux coordinates, domain decomposition. Designed for parallelization.
- Implicit time step, preconditioned conjugate gradients. Direct solution within blocks, CG over blocks.
- Web page: <http://www.nersc.gov/research/Nimrod>  
User Name: mhd, Password: www4mhd.

## Two-Fluid Equations

$$\frac{\partial n_j}{\partial t} + \nabla \cdot (n_j \mathbf{v}_j) = 0$$

$$\begin{aligned}\rho_j \left( \frac{\partial \mathbf{v}_j}{\partial t} + \mathbf{v}_j \cdot \nabla \mathbf{v}_j \right) + \nabla P_j + \nabla \cdot \Pi_j &= n_j q_j \left( \mathbf{E} + \frac{1}{c} \mathbf{v}_j \times \mathbf{B} \right) + \mathbf{R}_j \\ \frac{3}{2} \left( \frac{\partial P_j}{\partial t} + \mathbf{v}_j \cdot \nabla P_j \right) + \frac{5}{2} P_j \nabla \cdot \mathbf{v}_j + \nabla \cdot \mathbf{q}_j + \Pi_j : \nabla \mathbf{v}_j &= Q_j\end{aligned}$$

## Maxwell's Equations

$$\nabla \cdot \mathbf{B} = \nabla \times \mathbf{E} + \frac{1}{c} \frac{\partial \mathbf{B}}{\partial t} = 0$$

$$\mathbf{B} = \nabla \times \mathbf{A} \quad \mathbf{E} = -\nabla \varphi - \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t}$$

$$\nabla^2 \mathbf{A} = -\frac{4\pi}{c} \mathbf{J}$$

$$\nabla \cdot \mathbf{A} = \nabla \cdot \mathbf{J} = 0$$

## Constitutive Equations

$$\mathbf{J} = \sum_j \mathbf{J}_j = \sum_j n_j q_j \mathbf{v}_j$$

$\mathbf{q}$  and  $\Pi$  derived from particle moments

$$\text{Finite Element Discretization}$$

$$\frac{\partial u}{\partial t} + \nabla \cdot \mathbf{F} = S$$

$$u(t,\mathbf{x})=u_i(t)\alpha_i(\xi(\mathbf{x}),\eta(\mathbf{x}))$$

$$\mathcal{L}\equiv\int d\mathbf{x}\left[\frac{\partial u}{\partial t}+\nabla\cdot\mathbf{F}-S\right]^2,\quad\frac{\delta\mathcal{L}}{\delta(\partial u/\partial t)}=0$$

$$(f,g) \equiv \int f(\mathbf{x})g(\mathbf{x})d\mathbf{x} = \int f(\xi,\eta)g(\xi,\eta)\mathcal{J}(\xi,\eta)d\xi d\eta$$

$$\mathcal{J}\equiv\frac{\partial x}{\partial\xi}\frac{\partial y}{\partial\eta}-\frac{\partial x}{\partial\eta}\frac{\partial y}{\partial\xi}$$

$$-(\alpha_i,\nabla\cdot\mathbf{F})=\int d\mathbf{x}\mathbf{F}\cdot\nabla\alpha_i=\int d\xi d\eta \mathcal{J}\left(\mathbf{F}\cdot\nabla\xi\frac{\partial\alpha_i}{\partial\xi}+\mathbf{F}\cdot\nabla\eta\frac{\partial\alpha_i}{\partial\eta}\right)$$

$$(\alpha_i,\alpha_j)\dot{u}_j=\int d\xi d\eta \mathcal{J}\left(S\alpha_i+\mathbf{F}\cdot\nabla\xi\frac{\partial\alpha_i}{\partial\xi}+\mathbf{F}\cdot\nabla\eta\frac{\partial\alpha_i}{\partial\eta}\right)$$

## EXACT CONSERVATION LAW

$$\frac{\partial u}{\partial t} + \nabla \cdot \mathbf{F} = 0$$

$$U(\Omega, t) \equiv \int_{\Omega} u(\mathbf{x}, t) \, d\mathbf{x}$$

$$\frac{dU(\Omega, t)}{dt} = - \int_{\partial\Omega} \mathbf{F} \cdot \hat{\mathbf{n}} \, d\mathbf{x}$$

## FINITE ELEMENT CONSERVATION LAW

$$u(\mathbf{x}, t) = u_i(t) \alpha_i(\mathbf{x}), \quad (f, g) \equiv \int_V f(\mathbf{x}) g(\mathbf{x}) \, d\mathbf{x}$$

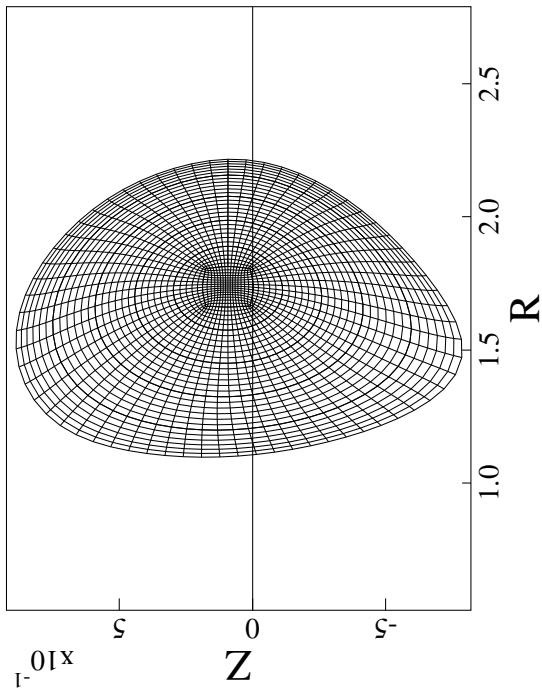
$$(\alpha_i, \alpha_j) \frac{du_j}{dt} = -(\alpha_i, \nabla \cdot \mathbf{F}) = \int_V \mathbf{F} \cdot \nabla \alpha_i \, d\mathbf{x}$$

$$U(\Omega, t) \equiv \int_{\Omega} u(\mathbf{x}, t) \varphi(\Omega, \mathbf{x}) \, d\mathbf{x}$$

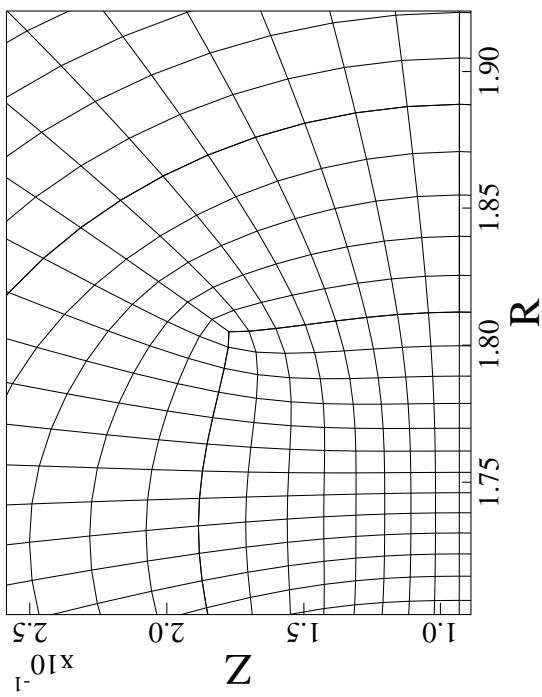
$\Omega$  bounded by grid lines,  $\varphi(\Omega, \mathbf{x}) = \sum_i \alpha_i(\mathbf{x}) \rightarrow 0$  on  $\partial\Omega$

$$\frac{dU(\Omega, t)}{dt} = \int_{\partial\Omega} \mathbf{F} \cdot \nabla \varphi(\Omega, \mathbf{x}) \, d\mathbf{x}$$

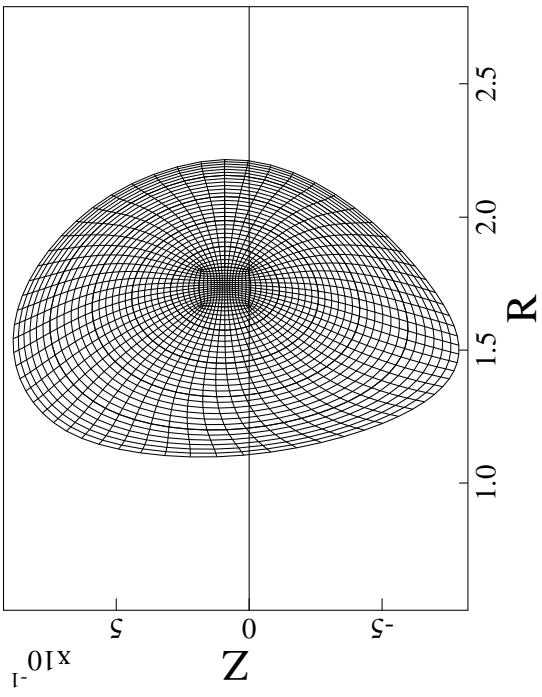
Nimrod Grid (Equal Arc - Smoothed)



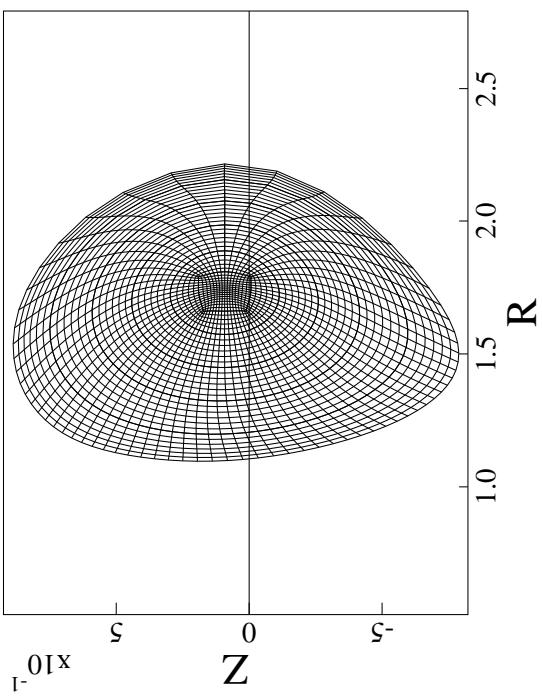
Nimrod Grid (Equal Arc - Smoothed)



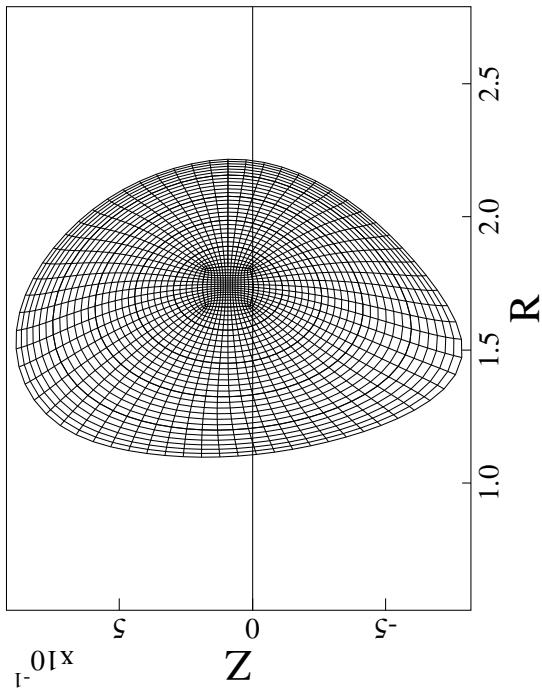
Nimrod Grid (Hamada - Smoothed)



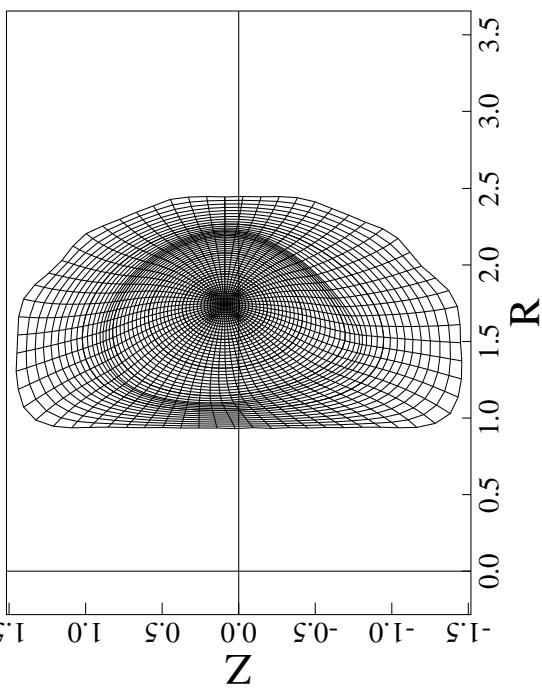
Nimrod Grid (PEST - Smoothed)



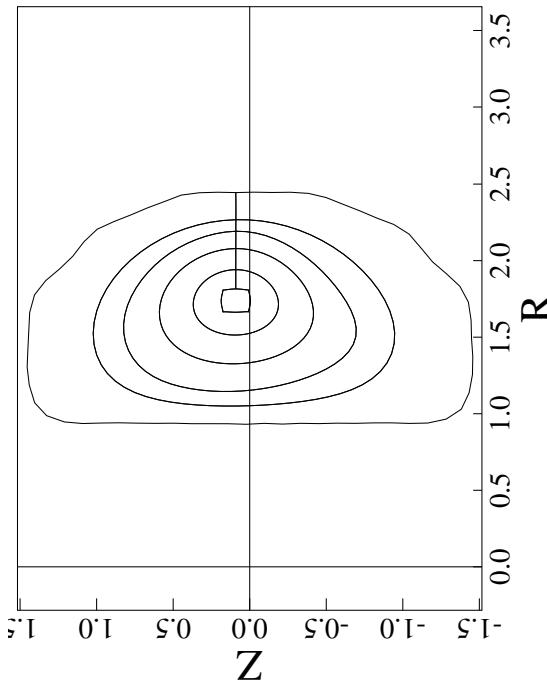
Nimrod Grid (Equal Arc - Smoothed)



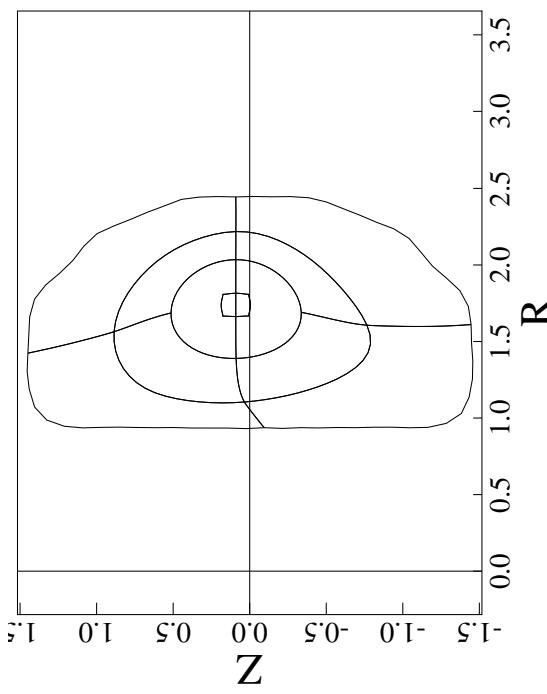
Nimrod Grid (Equal Arc - Smoothed)



Nimrod Grid Blocks



Nimrod Grid Blocks



## Spectral Pollution

- Gruber, Rappaz, and others have shown that finite element discretization of the ideal MHD stability problem can lead to spectral pollution: numerical eigenvalues that do not correspond to correct eigenvalues.
- The cause of spectral pollution is inaccuracy in representing the conditions:

$$\nabla \cdot \xi = 0, \quad \nabla \cdot \xi_{\perp} = 0, \quad \mathbf{B} \cdot \nabla f = 0$$

- To avoid spectral pollution, Gruber *et al.* use hybrid finite elements: different piecewise polynomial representations of the same physical quantity in different terms of the variational.
- This has several disadvantages:
  - The need for straight field line flux coordinates.
  - Compromise of the variational nature of the problem.
- Jaun showed that expressing the problem in terms of scalar and vector potentials  $\mathbf{A}$  and  $\varphi$  can avoid spectral pollution in the case of vacuum light waves.
- We have generalized Jaun's proof to the case of MHD waves in a uniform medium.
- Work is in progress on extending this work to include the effects of an implicit time step.

## Cold Linear Alfvén Waves, Potential Formulation

$$\mathbf{E} = -\nabla\varphi - \frac{1}{c}\frac{\partial\mathbf{A}}{\partial t}, \quad \mathbf{B} = \mathbf{B}_0 + \nabla \times \mathbf{A}, \quad \hat{\mathbf{b}} \equiv \mathbf{B}_0/B_0, \quad \nabla \cdot \mathbf{A} = 0 \quad (1)$$

$$\mathbf{E} + \frac{1}{c}\mathbf{v} \times \mathbf{B} = 0, \quad \mathbf{v} = \frac{1}{B}\hat{\mathbf{b}} \times \left( \frac{\partial\mathbf{A}}{\partial t} + c\nabla\varphi \right) + \mathbf{v}_{\parallel}, \quad \frac{1}{c}\frac{\partial A_{\parallel}}{\partial t} + \hat{\mathbf{b}} \cdot \nabla\varphi = 0 \quad (2)$$

$$\rho\frac{\partial\mathbf{v}}{\partial t} = \frac{1}{c}\mathbf{J} \times \mathbf{B}, \quad \mathbf{J} = \frac{\rho c}{B^2}\hat{\mathbf{b}} \times \left[ \hat{\mathbf{b}} \times \left( \frac{\partial^2\mathbf{A}}{\partial t^2} + c\nabla\frac{\partial\varphi}{\partial t} \right) \right] + \mathbf{J}_{\parallel}, \quad \frac{\partial v_{\parallel}}{\partial t} = 0 \quad (3)$$

$$\nabla \cdot \mathbf{J} = \nabla \cdot \left\{ \frac{\rho c}{B^2}\hat{\mathbf{b}} \times \left[ \hat{\mathbf{b}} \times \left( \frac{\partial^2\mathbf{A}}{\partial t^2} + c\nabla\frac{\partial\varphi}{\partial t} \right) \right] \right\} + \mathbf{B} \cdot \nabla \left( \frac{J_{\parallel}}{B} \right) = 0 \quad (4)$$

$$\nabla \times (\nabla \times \mathbf{A}) = -\nabla^2\mathbf{A} = \left( \frac{4\pi\rho}{B^2} \right)\hat{\mathbf{b}} \times \left[ \hat{\mathbf{b}} \times \left( \frac{\partial^2\mathbf{A}}{\partial t^2} + c\nabla\frac{\partial\varphi}{\partial t} \right) \right] + \frac{4\pi}{c}\mathbf{J}_{\parallel} \quad (5)$$

$$f(\mathbf{x}, t) = f_0 \exp(i\mathbf{k} \cdot \mathbf{x} - i\omega t), \quad c_A^2 \equiv \frac{B^2}{4\pi\rho}, \quad \mathbf{u} \equiv [A_x, A_y, A_z, \varphi, 4\pi J_{\parallel}/c]^T, \quad \mathbf{D} \cdot \mathbf{u} = 0 \quad (6)$$

$$[k^2\mathbf{I} - \omega^2/c_A^2(\mathbf{I} - \hat{\mathbf{b}}\hat{\mathbf{b}})] \cdot \mathbf{A} + \omega c/c_A^2 \mathbf{k} \cdot (\mathbf{I} - \hat{\mathbf{b}}\hat{\mathbf{b}})\varphi - \hat{\mathbf{b}}4\pi J_{\parallel}/c = 0, \quad \omega A_{\parallel}/c - k_{\parallel}\varphi = 0, \quad (7)$$

$$\begin{pmatrix} k^2 + (b_x^2 - 1)\frac{\omega^2}{c_A^2} & b_x b_y \frac{\omega^2}{c_A^2} & b_x b_z \frac{\omega^2}{c_A^2} & (k_x - b_x k_{\parallel}) \frac{\omega c}{c_A^2} & -b_x \\ b_x b_y \frac{\omega^2}{c_A^2} & k^2 + (b_y^2 - 1)\frac{\omega^2}{c_A^2} & b_y b_z \frac{\omega^2}{c_A^2} & (k_y - b_y k_{\parallel}) \frac{\omega c}{c_A^2} & -b_y \\ b_x b_z \frac{\omega^2}{c_A^2} & b_y b_z \frac{\omega^2}{c_A^2} & k^2 + (b_z^2 - 1)\frac{\omega^2}{c_A^2} & (k_z - b_z k_{\parallel}) \frac{\omega c}{c_A^2} & -b_z \\ (k_x - b_x k_{\parallel}) \frac{\omega^2}{c_A^2} & (k_y - b_y k_{\parallel}) \frac{\omega^2}{c_A^2} & (k_z - b_z k_{\parallel}) \frac{\omega^2}{c_A^2} & -(k^2 - k_{\parallel}^2) \frac{\omega c}{c_A^2} & k_{\parallel} \\ -b_x \frac{\omega}{c} & -b_y \frac{\omega}{c} & -b_z \frac{\omega}{c} & 0 & 0 \end{pmatrix} \quad (8)$$

$$D \equiv \det \mathbf{D} = -k^4(\omega^2/c_A^2 - k^2)(\omega^2/c_A^2 - k_{\parallel}^2) = 0 \quad (9)$$

## Basis Function Expansion

$$\nabla^2 \mathbf{A} - \frac{c}{c_A^2} \frac{\partial}{\partial t} \left( \mathbf{I} - \hat{\mathbf{b}}\hat{\mathbf{b}} \right) \cdot \left( \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} + \nabla \varphi \right) + \frac{4\pi}{c} J_{\parallel} \hat{\mathbf{b}} = 0, \quad (10)$$

$$\nabla \cdot \left[ \frac{c^2}{c_A^2} \frac{\partial}{\partial t} \left( \mathbf{I} - \hat{\mathbf{b}}\hat{\mathbf{b}} \right) \cdot \left( \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} + \nabla \varphi \right) \right] - 4\pi \hat{\mathbf{b}} \cdot \nabla J_{\parallel} = 0, \quad \hat{\mathbf{b}} \cdot \left( \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} + \nabla \varphi \right) = 0$$

$$\begin{aligned} \mathcal{L} \equiv & \int dt \int d\mathbf{x} \left\{ \frac{\partial}{\partial t} \left[ \nabla \mathbf{A} \right]^2 + \frac{c^2}{c_A^2} \left( \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} + \nabla \varphi \right) \cdot \left( \mathbf{I} - \hat{\mathbf{b}}\hat{\mathbf{b}} \right) \cdot \left( \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} + \nabla \varphi \right) \right] \\ & - 4\pi \left[ \left( \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} + \nabla \varphi \right) \cdot \hat{\mathbf{b}}\hat{\mathbf{b}} \cdot \mathbf{J} + \mathbf{J} \cdot \hat{\mathbf{b}}\hat{\mathbf{b}} \cdot \left( \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} + \nabla \varphi \right) \right] \} \end{aligned} \quad (11)$$

$$\frac{\delta \mathcal{L}}{\delta (\partial \mathbf{A} / \partial t)} = \frac{\delta \mathcal{L}}{\delta \varphi} = \frac{\delta \mathcal{L}}{\delta J_{\parallel}} = 0 \quad (12)$$

$$\mathbf{A}(\mathbf{x}, t) = \sum_i \mathbf{A}_i(t) \alpha_i(\mathbf{x}), \quad \varphi(\mathbf{x}, t) = \sum_i \varphi_i(t) \alpha_i(\mathbf{x}), \quad J_{\parallel}(\mathbf{x}, t) = \sum_i J_i(t) \alpha_i(\mathbf{x}) \quad (13)$$

$$\mathbf{A}_i = \mathbf{A}_0 \exp[i(\mathbf{k} \cdot \mathbf{x}_i - \omega t)], \quad \varphi_i = \varphi_0 \exp[i(\mathbf{k} \cdot \mathbf{x}_i - \omega t)], \quad J_i = J_0 \exp[i(\mathbf{k} \cdot \mathbf{x}_i - \omega t)] \quad (14)$$

$$\kappa \equiv \frac{\sum_j \exp[i\mathbf{k} \cdot (\mathbf{x}_j - \mathbf{x}_i)] \int \alpha_i \nabla \alpha_j d\mathbf{x}}{i \sum_j \exp[i\mathbf{k} \cdot (\mathbf{x}_j - \mathbf{x}_i)] \int \alpha_i \alpha_j d\mathbf{x}}, \quad \mathbf{\kappa} \equiv -\frac{\sum_j \exp[i\mathbf{k} \cdot (\mathbf{x}_j - \mathbf{x}_i)] \int \nabla \alpha_i \nabla \alpha_j d\mathbf{x}}{\sum_j \exp[i\mathbf{k} \cdot (\mathbf{x}_j - \mathbf{x}_i)] \int \alpha_i \alpha_j d\mathbf{x}} \quad (15)$$

$$(\text{tr } \mathbf{\kappa}) \mathbf{A}_0 - \frac{\omega c}{c_A^2} \left( \mathbf{I} - \hat{\mathbf{b}}\hat{\mathbf{b}} \right) \cdot \left( \frac{\omega}{c} \mathbf{A}_0 - \kappa \varphi_0 \right) - \frac{4\pi}{c} J_0 \hat{\mathbf{b}} = 0,$$

$$\frac{\omega c^2}{c_A^2} \left[ \frac{\omega}{c} \kappa \cdot (\mathbf{I} - \hat{\mathbf{b}}\hat{\mathbf{b}}) \cdot \mathbf{A}_0 - \mathbf{\kappa} : (\mathbf{I} - \hat{\mathbf{b}}\hat{\mathbf{b}}) \varphi_0 \right] - 4\pi \hat{\mathbf{b}} \cdot \kappa J_0 = 0, \quad \hat{\mathbf{b}} \cdot \left( \frac{\omega}{c} \mathbf{A}_0 - \kappa \varphi_0 \right) = 0 \quad (16)$$

## Discretized Dispersion Relation

$$\mathbf{D} \equiv \begin{pmatrix} \operatorname{tr} \mathbf{K} + (b_x^2 - 1) \frac{\omega^2}{c_A^2} & b_x b_y \frac{\omega^2}{c_A^2} & b_x b_z \frac{\omega^2}{c_A^2} & (\kappa_x - b_x \kappa_{\parallel}) \frac{\omega c}{c_A^2} & -b_x \\ b_x b_y \frac{\omega^2}{c_A^2} & \operatorname{tr} \mathbf{K} + (b_y^2 - 1) \frac{\omega^2}{c_A^2} & b_y b_z \frac{\omega^2}{c_A^2} & (\kappa_y - b_y \kappa_{\parallel}) \frac{\omega c}{c_A^2} & -b_y \\ b_x b_z \frac{\omega^2}{c_A^2} & b_y b_z \frac{\omega^2}{c_A^2} & \operatorname{tr} \mathbf{K} + (b_z^2 - 1) \frac{\omega^2}{c_A^2} & (\kappa_z - b_z \kappa_{\parallel}) \frac{\omega c}{c_A^2} & -b_z \\ (\kappa_x - b_x \kappa_{\parallel}) \frac{\omega^2}{c_A^2} & (\kappa_y - b_y \kappa_{\parallel}) \frac{\omega^2}{c_A^2} & (\kappa_z - b_z \kappa_{\parallel}) \frac{\omega^2}{c_A^2} & -(\mathbf{I} - \hat{\mathbf{b}}\hat{\mathbf{b}}) : \mathbf{K}_{\frac{\omega c}{c_A^2}} & \kappa_{\parallel} \\ -b_x \frac{\omega}{c} & -b_y \frac{\omega}{c} & -b_z \frac{\omega}{c} & 0 & 0 \end{pmatrix} \quad (17)$$

$$D \equiv \det \mathbf{D} = \left[ \frac{\omega^2}{c_A^2} - (\operatorname{tr} \mathbf{K}) \right] \left\{ \frac{\omega^4}{c_A^4} (\mathbf{I} - \hat{\mathbf{b}}\hat{\mathbf{b}}) : (\mathbf{K} - \kappa \kappa) - \frac{\omega}{c_A^2} (\operatorname{tr} \mathbf{K}) \left[ (\operatorname{tr} \mathbf{K}) - \hat{\mathbf{b}}\hat{\mathbf{b}} : (\mathbf{K} - \kappa \kappa) \right] + (\kappa \cdot \hat{\mathbf{b}})^2 (\operatorname{tr} \mathbf{K})^2 \right\} = 0 \quad (18)$$

$$\begin{aligned} \frac{\omega^2}{c_A^2} &= (\operatorname{tr} \mathbf{K}), \\ &\approx (\kappa \cdot \hat{\mathbf{b}})^2 (\operatorname{tr} \mathbf{K}) \left[ (\operatorname{tr} \mathbf{K}) - \hat{\mathbf{b}}\hat{\mathbf{b}} : (\mathbf{K} - \kappa \kappa) \right]^{-1}, \\ &\approx (\operatorname{tr} \mathbf{K}) \left[ (\operatorname{tr} \mathbf{K}) - \hat{\mathbf{b}}\hat{\mathbf{b}} : (\mathbf{K} - \kappa \kappa) \right] \left[ (\mathbf{I} - \hat{\mathbf{b}}\hat{\mathbf{b}}) : (\mathbf{K} - \kappa \kappa) \right]^{-1} \end{aligned} \quad (19)$$

## Evaluation of $\kappa$ and $\mathbf{K}$

$$\kappa = \frac{\mathcal{I}_1}{\mathcal{I}_0}, \quad \mathbf{K} = \frac{\mathcal{I}_2}{\mathcal{I}_0} \quad (20)$$

$$\begin{aligned} \mathcal{I}_0 &\equiv \sum_j \exp[i\mathbf{k} \cdot (\mathbf{x}_j - \mathbf{x}_i)] \int \alpha_i \alpha_j d\mathbf{x} \\ &= (4 + 2 \cos k_x h_x + 2 \cos k_y h_y + \cos k_x h_x \cos k_y h_y) h_x h_y / 9 \end{aligned} \quad (21)$$

$$\mathcal{I}_1 \equiv -i \sum_j \exp[i\mathbf{k} \cdot (\mathbf{x}_j - \mathbf{x}_i)] \int \alpha_i \nabla \alpha_j d\mathbf{x} \quad (22)$$

$$\begin{aligned} &= [\hat{\mathbf{x}}(6 + 3 \cos k_y h_y) \sin k_x h_x / h_x + \hat{\mathbf{y}}(6 + 3 \cos k_x h_x) \sin k_y h_y / h_y \\ &+ \hat{\mathbf{z}}(4 + 2 \cos k_x h_x + 2 \cos k_y h_y + \cos k_x h_x \cos k_y h_y) k_z] h_x h_y / 9 \end{aligned}$$

$$\mathcal{I}_2 \equiv - \sum_j \exp[i\mathbf{k} \cdot (\mathbf{x}_j - \mathbf{x}_i)] \int \nabla \alpha_i \nabla \alpha_j d\mathbf{x}$$

$$\begin{aligned} &= [\hat{\mathbf{x}}\hat{\mathbf{x}}(12 + 6 \cos k_y h_y)(1 - \cos k_x h_x) / h_x^2 + \hat{\mathbf{y}}\hat{\mathbf{y}}(12 + 6 \cos k_x h_x)(1 - \cos k_y h_y) / h_y^2 + \hat{\mathbf{z}}\hat{\mathbf{z}}k_z^2 \\ &+ (\hat{\mathbf{x}}\hat{\mathbf{z}} + \hat{\mathbf{z}}\hat{\mathbf{x}})(6 + 3 \cos k_y h_y)(\sin k_x h_x / h_x) k_z + (\hat{\mathbf{y}}\hat{\mathbf{z}} + \hat{\mathbf{z}}\hat{\mathbf{y}})(6 + 3 \cos k_x h_x)(\sin k_y h_y / h_y) k_z \\ &+ 9(\hat{\mathbf{x}}\hat{\mathbf{y}} + \hat{\mathbf{y}}\hat{\mathbf{x}})(\sin k_x h_x / h_x)(\sin k_y h_y / h_y)] h_x h_y / 9 \end{aligned} \quad (23)$$

$$\begin{aligned} \hat{\mathbf{b}}\hat{\mathbf{b}} : (\mathbf{K} - \kappa\mathbf{K}) &= (b_x^2 k_x^4 h_x^2 + b_y^2 k_y^4 h_y^2) / 12 + \dots, \\ (\mathbf{l} - \hat{\mathbf{b}}\hat{\mathbf{b}}) : (\mathbf{K} - \kappa\mathbf{K}) &= [(1 - b_x^2) k_x^4 h_x^2 + (1 - b_y^2) k_y^4 h_y^2] / 12 + \dots \end{aligned} \quad (24)$$